MSTe NEWS
May 2019
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INSIDE

Los Alamos NATIONAL LABORATORY EST.1943

To study polymer degradation, Dali Yang uses comprehensive techniques and instrumentation. Yang, shown here in her lab in the Target Fabrication Facility, employs multi-detection gel permeation chromatography to study the molecular weight, distribution, and structure of a degraded polymer and to investigate the interaction between the degraded polymer and organic solvent.
Photo credit: Kevin Sutton (XIT-TSS)

Dali Yang

Persistently pursuing advances in polymer science

"My multidisciplinary knowledge and training help me observe overlooked details and ask fundamental questions about aging behavior of materials that often lead to new and exciting findings."

In her 20 years at Los Alamos National Laboratory, Dali Yang said she has "never been bored." She has worked on projects funded by Stockpile Stewardship and DOE's Fossil Energy and Energy Efficiency and Renewable Energy offices, the Department of Homeland Security, and Los Alamos's Laboratory Directed Research and Development program.

Yang, a member of the Thin Films and Coatings team in Engineered Materials (MST-7) studies polymers and their composites—materials that she finds fascinating and complex and that are "integral to our daily lives," she said. "Polymers touch almost every aspect of our modern life."

These versatile materials—found in items ranging from clothes to electronic gadgets and storage containers—have allowed Yang to perform a range of research aimed at improving polymer functionality and stability for eco-sustainability.

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From David's desk . . .

In an effort to improve the effectiveness of our communications both internal and external to the Lab, the MST management team asked you to participate in a survey on communications. Detailed results of the survey can be found on our internal web site at int.lanl.gov/org/ddste/aldps/mst/index.shtml (under the "News!" tab), but I will try to summarize high points here.

Beyond our traditional means of communicating our science accomplishments via publications and conferences, you noted that web sites and videos were the next two preferred means of communicating both within the Lab and externally. We thought perhaps that social media might have been more popular, but the survey did not indicate that. This is useful feedback to obtain so that we don't put a significant amount of effort in publicizing our accomplishments via that platform. We have decided that we will put some effort in updating and modernizing both our external and internal web pages, which should address comments several of you made relative to information and contacts that were out of date. Since we already put significant effort into creating highlights both for *MST e-News* and institutional highlights, we plan to regularly repurpose that content on our web pages to help them stay current while also reducing the amount of extra work.

We are also piloting an initiative creating short informational videos to help a broader audience connect with the type of science and technology we perform in MST. Our goal is to create short, three-minute videos to quickly help the audience understand the importance and impact of the research being performed in MST. These videos will be showcased on our external web site with links to further information. Initially, Blas Uberuaga will be creating a series of videos for his Basic Energy Sciences, Energy Frontier Research Center program, FUTURE. If you have a highlight or topic that you think would be a good candidate for a short video, please let me know and we can help provide the resources to produce it.

Lastly, many of you were unaware that we had developed MST Division and group brochures as well as accompanying brochures on the LANL materials strategy, but if you had them you would use them for sharing with our recruits, external colleagues, and program sponsors. We will be making several folders available in each group office for you to obtain and share as you see fit. Let us know if there is any other information that you think would be good to include in these informational folders. This will be a project for one of our summer students, so these folders should be available in the early summer timeframe.

MST Division continues to be highly innovative and productive and we should celebrate our successes. Having an effective communication plan will help a much broader audience (internal and external) understand the value that MST scientists bring to our missions and programs. Thanks again for participating in the survey and helping us create an effective communications strategy.

MST Division Leader David Teter

"*MST Division continues to be highly innovative and productive and we should celebrate our successes.*"

Yang cont.

Yang earned her master's degree in chemical engineering from Stevens Institute of Technology in New Jersey and PhD in chemistry from the University of California, Los Angeles. Her engineering and science training allows her to approach problems considering industrial practicability and scientific feasibility.

Yang first made an impact in the fields of renewable energy and energy recovery as a Laboratory staff member. Leading a team of scientists, engineers, and technologists from Los Alamos, Chevron, SpectrumLab, and the University of Minnesota, she engineered polymeric-based hollow fibers into novel packing materials used in olefin/paraffin distillation processes. The invented technology significantly enhances the separation efficiency, will save substantial energy, and reduces harmful emissions in distillation industries.

"This idea, suggested by a number of others, never looked practical," said colleague E. L. Cussler (University of Minnesota). "The LANL team has made it considerably more viable." The technology was successfully demonstrated from a bench-top to a pilot-plant scale and was awarded a U.S. patent.

Yang's multidisciplinary knowledge allows her to combine experimental and theoretical approaches to solve complex problems. During a CO_2 sequestration project, she oversaw the entire experimental operation—from process design to continuous flow reactor construction to the reactor testing. She also developed numerical programs to process a large set of raw data, obtaining thermodynamic, kinetic, and hydrodynamic parameters for the clathrate hydrate formation process under industrial operation conditions. The project was recognized with an R&D 100 Award.

"While contributing to our large technical projects, Dali has clearly demonstrated the ability to develop innovative solutions based on sound theories and approaches," said Robert Currier (Physical Chemistry and Applied Spectroscopy, C-PCS).

To support the Lab's stockpile stewardship mission, Yang leads projects studying polymer stability and degradation. In one, she collaborates with high explosives scientists from across the Laboratory, performing artificial aging experiments and investigating the degradation mechanisms of polymers. These mechanisms will be implemented in computational models simulating the complex reactions within the weapon system. Yang said this multidisciplinary work is one of her favorite parts of working at the Lab.

To fulfill her team's role in determining the fitness of the nation's deterrent, she and her colleagues test polymeric materials by putting them in confined chambers and changing environmental aspects like temperature and humidity to mimic real application conditions. A typical experiment that Yang designs will take 3-6 years to complete. Even then, with the resulting data in hand, she continues to maintain a questioning attitude, acknowledging that the more she learns, the more she realizes how much she doesn't understand.

The complexity and lengthy timeframe required for her work is why Yang stresses the importance of carefully designing and executing experiments from the outset. She attributes her success to this attitude and she hopes to pass it on to the students and young colleagues she mentors. "I try to help them understand why details matter and persistence is critical," she said. "Don't give up so easily and remember that systematic work is important."

Yang takes her mentor role seriously, as she remembers the lessons that others taught her. "I like mentoring because of the way I grew as a senior scientist here," she said. "A lot of people lent a hand, so I try to have a lot of patience with students. I want to make sure they can learn a lot during their time with me."

"My multidisciplinary knowledge and training help me observe overlooked details and ask fundamental questions about the aging behavior of materials that often lead to new and exciting findings," she said. The sophisticated, systematic, and diligent experiments she and her colleagues perform are leading to "innovations in both material science and polymer chemistry, which is really challenging yet highly exciting and rewarding."

MST e NEWS

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To submit news items or for more information, contact Karen Kippen, ALDPS Communications, at 505-606-1822, or aldps-comm@lanl.gov.

For past issues, see www.lanl.gov/org/ddste/aldps/mst-e-news.php.

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NNSA National Nuclear Security Administration

MST staff in the news

Stuart Maloy named UNM Nuclear Engineering National Laboratory Professor

Stuart Maloy has been appointed a National Laboratory Professor in the University of New Mexico Department of Nuclear Engineering. The National Lab Professorship enables distinguished scientists and engineers affiliated with Los Alamos National Laboratory and Sandia National Laboratories to assume faculty appointments as professors within academic departments at the University of New Mexico.

Maloy was chosen because of his extensive background in studying radiation effects in materials. His responsibilities include developing research collaborations, serving as co-principal investigator on proposals, helping with academic courses, and recruiting and advising students.

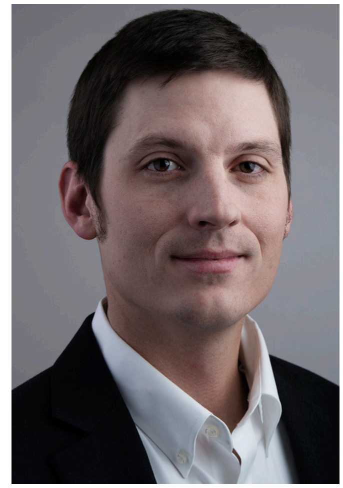
Maloy is deputy group leader for Materials Science in Radiation and Dynamics Extremes (MST-8) and has been at the Laboratory for nearly 30 years. He earned a PhD in materials science from Case Western Reserve University and is a registered professional engineer in metallurgy. He has more than 200 peer-reviewed technical publications with over 2,500 citations and an H-index of 28.

Technical contact: Stuart Maloy

Topher Matthews recognized with DOE Fuel Cycle R&D Excellence award

Topher Matthews received a DOE Fuel Cycle R&D Excellence award for his work developing simulations of nuclear fuels at the engineering scale.

The awards, given by the DOE Fuel Cycle R&D program to early-to-mid career scientists from five national laboratories, were presented during a broad-scope American Nuclear Society (ANS) technical session, part of the ANS Winter Meeting in Orlando. The session was designed to disseminate information and spur discussion on a number of topics, including fuel development and separation, advanced reactor systems, material protection, and modeling/simulations in related areas. It highlighted the recent R&D progress by these early-to-mid career scientists in the DOE's Nuclear Technology Research and Development program.



As an award recipient, Matthews (Materials Science in Radiation and Dynamics Extremes, MST-8) was invited to present his work on advanced BISON models.

Matthews uses atomistic data from MST-8 to generate codes that compare experimental and post-irradiation examination data. BISON is a fuel performance code, and Matthews serves as the lead of a Los Alamos team that supports the Advanced Fuels Campaign at Idaho National Laboratory (INL) with advanced fuel performance models and capabilities.

National Technical Director for the Advanced Fuels Campaign and INL scientist Steve Hayes nominated Matthews for the award. To commemorate the award, Matthews was presented with a piece of graphite that was used in the CP-1, the world's first nuclear reactor, a project led by Enrico Fermi.

Matthews received his PhD in nuclear engineering from Oregon State University and joined the Laboratory in 2015. He said he sees his work as contributing to the progress of nuclear energy as a "green" technology. His phenomenological models and computer simulations aid in the understanding, development, and application of advanced materials that will drive the advancement of fission energy and fast reactors. His work supports the Lab's Energy Security mission and Materials for the Future science pillar.

Technical contact: Topher Matthews

Saryu Fensin receives AIME Hardy Award

Saryu Fensin is a co-recipient of the 2019 AIME Robert Lansing Hardy Award, which recognizes talented scientists under the age of 35 in the fields of metallurgy and materials science. The Minerals, Metals, and Materials Society (TMS) gives this award in recognition of the scientist for his or her "exceptional promise of a successful career."

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MST staff cont.

Fensin (Materials Science in Radiation and Dynamics Extremes, MST-8) uses both experimental and computational methods to study the relationship between a material's microstructure and its performance in extreme environments, like high strain and temperature.

She has held many leadership positions within TMS, including serving on the Young Professionals, Professional Development, Diversity, and Mechanical Behavior of Materials committees. She previously received the TMS Young Leaders International Scholar—Japanese Institute of Metals Award and the TMS Young Leaders Professional Development Award.

Fensin earned her PhD in materials science and engineering from the University of California, Davis, and joined the Laboratory in 2010 as a postdoctoral researcher. She is a staff member on MST-8's Dynamic and Quasistatic Loading Experimental Team, where she is the principal investigator on multiple projects, including an effort to understand damage and failure in materials funded by Experimental Sciences Campaign 2 (LANL Program Manager Dana Dattelbaum) and an effort to study plutonium aging funded by Experimental Sciences Campaign 1 (LANL Program Manager Ray Tolar).

The award, established by Arthur Hardy in memory of his late son who showed promise in the field of physical metallurgy, was presented at the recent TMS-AIME Annual Awards Ceremony in San Antonio.

Technical contact: Saryu Fensin

Rusty Gray receives George E. Duvall Shock Compression Science Award

George (Rusty) T. Gray III (Materials Science in Radiation and Dynamics Extremes, MST-8) is the 2019 recipient of the American Physical Society's (APS) George E. Duvall Shock Compression Science Award. This award is given to an APS member who has contributed to understanding condensed matter and nonlinear physics through shock compression.

Gray was cited for "pioneering contributions in dynamic constitutive and damage response of materials; for leadership in developing programs and tools to advance our understanding of materials and structures in response to high-strain-rate and shock deformation; and for leadership in the technical community." This Society-level award represents one of the highest recognitions for contributions to the field of physics by a member of the physics community.

For more than 30 years, Gray has made essential contributions to the Laboratory's Stockpile Stewardship efforts. He was recently selected to serve on the new National Academy of Sciences board on Army R&D, which focuses on emerging threats, and in 2017 was elected to the National Academy of Engineering.

His research focuses on the structure–property relationship during high strain rate and shock deformation of defense-relevant materials. A cross-disciplinary scientist with a PhD in metallurgical engineering from Carnegie Mellon University, Gray combines dynamic experiments, post-shock material studies, and cutting-edge theoretical modeling. An example of Gray's pioneering work is the use of "soft" shock recovery experiments for the study of post-shock material response.

Shock compression and shock-wave deformation are especially critical in the absence of underground nuclear testing. Gray's contributions in these areas support the Laboratory's national security science mission by bringing insight into how materials respond under high strain rate and high shock loading.

Gray is the fifth Laboratory recipient of this APS award and the eleventh national laboratory recipient. He is the second winner who is also a member of the National Academy of Engineering. Gray will be presented with the award at the June Shock Compression of Condensed Matter conference in Portland, Oregon.

Technical contact: Rusty Gray

Celebrating service

Congratulations to the following MST Division employees celebrating recent service anniversaries:

Cynthia Sandoval, MST-7 .... 35 years
Stuart Maloy, MST-8 .... 30 years
Miquela Sanchez, MST-7 .... 30 years
Bjorn Clausen, MST-8 .... 20 years
Ernesto Gallegos, MST-16 .... 20 years
Brett Robinson, MST-16 .... 15 years
Veronica Livescu, MST-8 .... 15 years
Theresa Quintana, MST-7 .... 15 years
Joseph Romero, MST-16 .... 15 years
Paul Tobash, MST-16 .... 10 years
Neliza Brito, MST-7 .... 5 years
Paul Donovan, MST-7 .... 5 years
Helen Milenski, MST-16 .... 5 years
Douglas Vodnick, MST-7 .... 5 years

Integrating complex functional materials with additive manufacturing

Engineering Materials (MST-7) researchers have developed a new three-dimensional printing technology to manufacture advanced materials with hierarchical architectures and engineered functionalities.

Their research capitalizes on the benefits of both additive manufacturing technology and nanomaterials chemistry to engineer new generations of "designer" materials for catalysis, weapons systems, separations, heat transfer, and beyond.

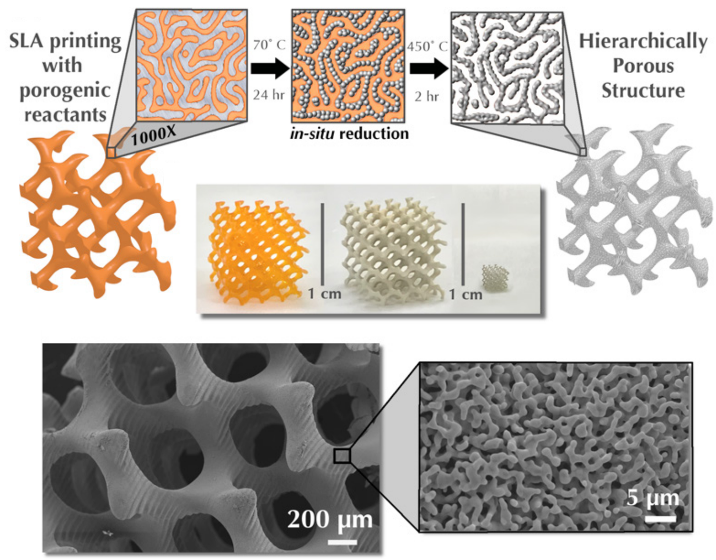
The work, for which several patents have been applied, "upgrades" traditional stereolithography by using self-assembly processes within printed objects, enabling nanoscale casting of metals, ceramics, oxides, and multi-phase composites (e.g., conductive polymers).

The technique also opens up stereolithography to new classes of polymers, including silicones, epoxies, and bioplastics that until now were not compatible with photochemical additive manufacturing techniques. The goal is to capitalize on the advantages of vat stereolithography (speed, high resolution, and scalability) while producing complex and high-performance materials across multiple length scales.

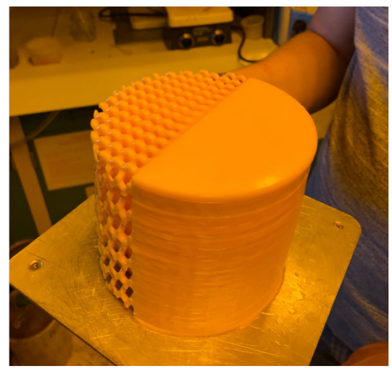
The research comprises several embodiments of an overarching R&D concept, which is to use polymerization-induced phase separation within a three-dimensional printed object to generate micro/meso-structures within its walls.

At this point a multitude of simple processing steps can be used to transform or modulate the material chemistry upon removal of fugitive components. These transformations can be achieved by in situ ion reduction, crosslinking of miscible monomers, or sol-gel chemistry, among other techniques.

The work supports the Laboratory's Energy Security mission area and its Materials for the Future science pillar by developing materials with a specific function and predictable performance, the key focus of the Lab's materials strategy.



Above: illustration and digital/scanning electron microscope images of production of a hierarchical nested-network porous silver monolithic via additive manufacturing. The bi-modal porosity is engineered across two widely separated length scales.

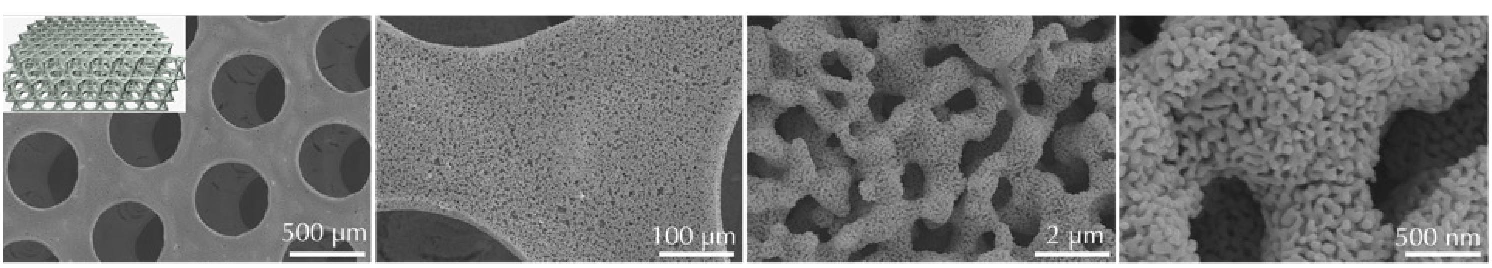


Right: large-scale objects possessing hierarchical nano-architectures and prescribed chemical functionalities can be readily manufactured using low-cost commercial three-dimensional printing equipment.

Facets of this research have been funded by several Laboratory Directed Research and Development Program Exploratory and Mission Foundation research projects, the Science Programs, the Stockpile Responsiveness Program, and the Enhanced Surveillance Program. This technology is being continually developed by Matt Lee, Nicholas Parra-Vasquez, and Kyle Cluff (MST-7).

Reference: U.S. Patent App. No. 16/265641 (2019).

Technical contact: Matt Lee



Scanning electron microscopy images of a nested-network gold material with three levels of engineered porosity.

Advantages of pyrochlore ($A_2B_2O_7$) amorphization in long-term actinide waste disposal

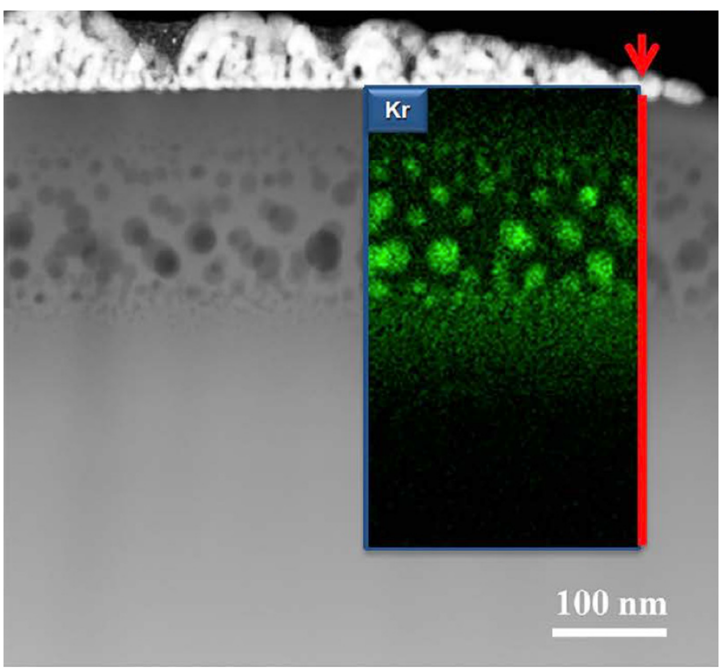
Retention of gaseous species in irradiated pyrochlores makes actinide waste more stable and immobilized

Lanthanide pyrochlores are a class of complex oxides that offer potential as a host matrix for nuclear waste forms of plutonium and related minor actinide materials. Given that actinide waste produces radiation, understanding the structure–property relationship of pyrochlores under such extreme conditions is key to evaluating their reliable, long-term performance for such an application.

One crucial relationship in a material destined for irradiation extremes is the ability to withstand or accommodate amorphization—the process of becoming non-crystalline. Previously, amorphization of waste matrix materials was considered a negative feature; however, new research by MST researchers on the amorphization of pyrochlores suggests otherwise.

Their results indicate that rapid amorphization of initially crystalline waste from materials with accumulated dose may not always be harmful. Their work also suggests new avenues for the design of materials to encapsulate and immobilize certain types of actinide materials.

Using a 200-kV Danfysik Research ion implanter at the Ion Beam Materials Laboratory at Los Alamos National Laboratory, the researchers implanted Kr^{2+} into two pyrochlore materials: $Gd_2Zr_2O_7$ (GZO) and $Gd_2Ti_2O_7$ (GTO). The addition of Kr^{2+} and the presence of radiation are expected to lead to large bubble formation, defects, and microcracking in the pyrochlores materials. Their research, which appeared in *Acta Materialia*, showed that GTO completely amorphized and resisted microcracking and gas release.



Z-contrast scanning transmission electron microscopy (STEM) image of irradiated GTO implanted with Kr^{2+} with an inset of a Kr energy-dispersive x-ray spectroscopy (EDS) map and a line marking where the EDS line scan was taken.

Their results indicate that amorphized GTO has an enhanced propensity to retain and accommodate gaseous species in actinide waste, thereby resisting microcracking caused by the gas bubbles. For long-term storage and immobilization of actinide material waste, irradiated GTO should be considered as a beneficial host matrix that will resist microcracking and defects over time.

Reference: "Potential benefit of amorphization in the retention of gaseous species in irradiated pyrochlores," *Acta Mat.* 164, 250–260 (2018).

Researchers: Terry Holesinger and Matthew Janish (Nuclear Materials Science, MST-16), James Valdez, Yongqiang Wang, and Blas Uberuaga (Materials Science in Radiation and Dynamics Extremes, MST-8).

This work, which supports the Laboratory's Energy Security mission and Materials for the Future science pillar, was funded by the U.S. DOE Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division under award 2013LANL8400.

Technical contacts: Terry G. Holesinger and James Valdez

Predicting damage and failure in additively manufactured tantalum

A team of researchers in Materials Science in Radiation and Dynamics Extremes (MST-8) has published well-received findings on the strength of additive manufactured (AM) tantalum. The work details the properties of AM-produced tantalum on different scales, including how microstructure and impurities within the material affect spall strength. The *Journal of Applied Physics* highlighted the work on its cover and as a feature article.

The AM process is attractive for many reasons, including its ability to construct complex geometries while reducing production time. It is particularly useful for applications requiring components that are costly in design and require few replicates, such as space and defense applications. However, these applications are particularly challenging as they encounter dynamic loading conditions such as ballistic impact and explosive loading. The stresses on these materials can range over several orders of magnitude.

For these reasons, the researchers demonstrated the differences between wrought tantalum and AM-constructed

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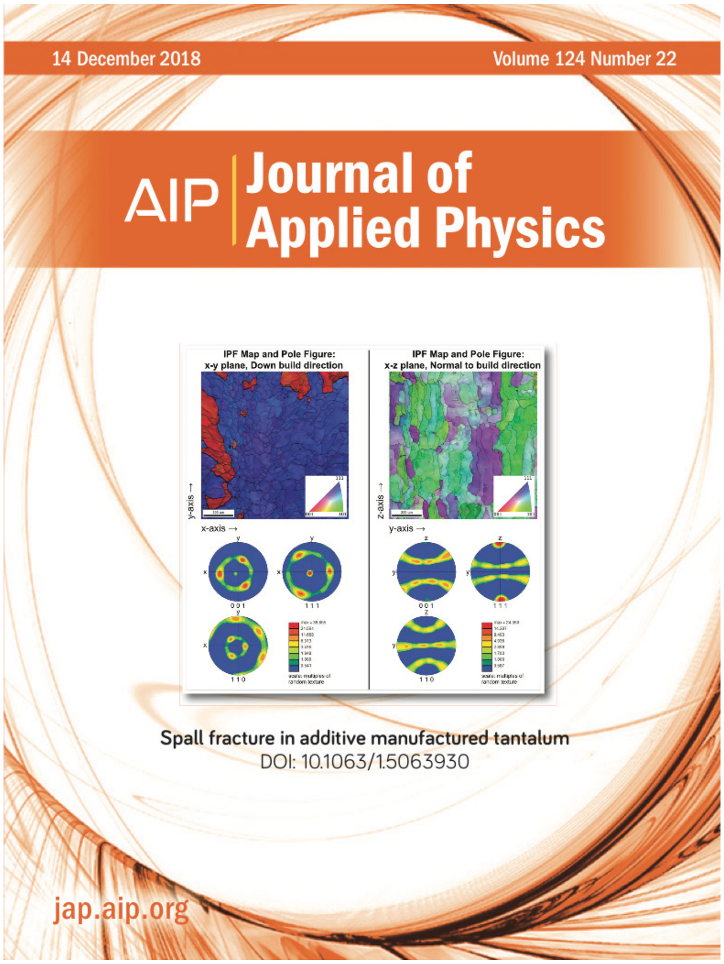
Predicting cont.



The cover of *J. Appl. Phys.* features a figure from the paper.

tantalum. Among other tests, they subjected the materials to a single-stage light-gas gun available in MST-8 coupled with recovery and post-mortem analysis of the sample to study spallation after projectile impact.

On a molecular scale, the team found that AM tantalum contained more impurities than its wrought counterpart and that its microstructure was highly anisotropic—the material is stronger in one direction than another. After stressing the materials by using the light-gas gun, they found that wrought tantalum nucleates voids into narrow lines, whereas the voids in AM tantalum still nucleated but were much more widely spread. They found that these molecular characteristics translated to performance differences at the macro scale.

Upon subjecting the samples to shock loading, the researchers found that AM tantalum had a higher Hugoniot elastic limit (dynamic yield strength) and a lower spall strength (resistance to dynamic tension) compared with wrought tantalum. They tested whether there was a difference in spall strength depending on the orientation of the loading direction and the build direction, but they found no strong trend.

Future efforts include implementing different additive manufacturing processes to see how a change in impurity content or manufacturing method affects the structure, properties, and performance of AM tantalum.

The work supports the Laboratory's Materials for the Future science pillar, including its defect and interfaces theme by working to tailor materials to enable controlled functionality and predictive performance, which is the central vision of the Laboratory's materials strategy. This work was funded through the Laboratory Directed Research and Development program.

Researchers: D. R. Jones, S. J. Fensin, B. G. Ndefru, D. T. Martinez, C. P. Trujillo, and G. T. Gray III (MST-8).

Reference: "Spall fracture in additive manufactured tantalum" *J. Appl. Phys*. 124, 225902 (2018).

Technical contact: David Jones

HeadsUP!

Distracted driving awareness

Every day, at least 9 Americans die and 100 are injured in distracted driving crashes.

Visual driving distractions cause you to take your eyes off the road. These distractions include
- checking your GPS or navigation system;
- looking to see what song is playing on the radio;
- searching for mirror or temperature controls; and
- looking for lost items on the floor of your vehicle.

Manual distractions are distractions that cause you to take your hands off of the wheel. These include
- eating, drinking, or smoking;
- checking your phone;
- adjusting the radio; and
- setting a destination in your vehicle's in-dash navigation system

Cognitive distractions take your focus and concentration away from driving. These include
- talking to passengers in the vehicle;
- encountering road rage;
- driving under the influence of drugs or alcohol; and
- driving while drowsy or fatigued.